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Micro-scale modelling of bovine cortical bone fracture: Analysis of crack propagation and microstructure using X-FEM

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ABSTRACT

Bone-fracture susceptibility is increased by factors such as bone loss, microstructure changes, and variations in material properties. Therefore, investigation of the effect of microstructure and material properties of bone on crack propagation in it and of its global response at macro-scale is important. A non-uniform distribution of osteons in a cortical bone tissue results in a localization of deformation processes. Such localization can affect bone's performance under external loads and initiate fracture or assist its propagation. Once the fracture initiates, that distribution can play an important role in the crack propagation process at micro-scale; subsequently, the global response at macro-scale could also be affected. In this study, a two-dimensional numerical (finite-element) fracture model for osteonal bovine cortical bone was developed with account for its microstructure using extended finite element method (X-FEM). The topology of a transverse-radial cross section of a bovine cortical bone was captured using optical microscopy. Mechanical properties for the bone's micro-structural features in the cross section were obtained with a use of the nanoindentation technique. Both the topology and nanoindentation data were used as input to the model formulated with the Abaqus finite-element software. The area, directly reflecting micro-scale information, was embedded into the region with homogenised properties of the cortical bone. Numerical simulations provide the macro-scale global response, crack propagation paths and distribution of maximum principal stress at the microscopic level for three different topologies – homogeneous, three-phase composite and four-phase composite model under tensile loading conditions.

The calculated stress fields for various cases of topologies demonstrate different patterns due to implementation of micro-structural features in the finite-element models, confirming an important role of the microstructure in the crack propagation scenarios. The suggested approach emphasizes the importance of micro-structural features, especially cement lines, in development of bone failure.

1. Introduction

Bone fractures have significant health, economic and social consequences. To plan prevention therapies and treatment strategies, scientific knowledge of bone fracture mechanisms is needed [1]. The failure process in a cortical bone tissue is affected by several factors, such as bone mineral density (bone loss), micro-structural changes, variations in its material properties and accumulation of microcracks [2,3]. Factors such as porosity, mineralization, orientation, diameters and spacing of collagen fibres and other aspects of histological structure strongly affect mechanical properties; they have effect on crack initiation and growth [4]. The effect of bone quantity on the mechanical behaviour and structural integrity of bone was established previously [5,6]; however, more in-depth investigations of the contributory effects of microstructure, material properties, and microcrack propagation are still required [3,7]. An improved understanding of bone's resistance to crack initiation and propagation can help in accessing bone fracture risk [8]. It is well known that damage occurs in both trabecular and cortical bones due to daily-activity loading regime [9]. Microdamage can be repaired by remodelling process; however, if the bone's repair mechanism is deficient, fragility fractures may result due to minor trauma, especially in ageing bone [10]. Experimentally, both the damage location and morphology in the form of linear microcracks were characterised [11–13]. Also, the relationship between the crack length and propagation in compact bone tested in cyclic fatigue under four-point bending was investigated [10]. It was found that if linear microcracks possess enough energy or the repairing system is deficient, they can propagate and lead to fracture.

Structurally, bone is a complex hierarchical composite. Histologically, bovine cortical bone is characterised as primary and secondary. During bone growth, primary bone is established on existing bone surfaces, such as circumferential lamellar bone underneath the perisosteal surface [10]. Blood vessels are

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surrounded by concentric lamellae known as primary osteons. Primary osteons are smaller, shorter, fewer in numbers and have no cement lines as compared to compact bone's secondary osteons [14]. Secondary osteons in compact bone result from absorption and replacement of old bone by new lamellar bone through remodelling process. Their shapes are round to ellipsoidal in radial-transverse cross-sections of cortical bones and form basic building blocks of the cortical bone tissue [10]. Their diameters vary between 100 and 400 μm and can be between 1 and 2 mm in length [15]. Each osteon comprises several lamellae surrounding a central Haversian canal and bounded by a so called *cement line* that separates one osteon from another and from the surrounding interstitial bone. The material properties of this weak thin amorphous interface – cement line – are not fully established yet [16]. Secondary compact bone can be considered as composite material [2,7]. In such a composite, osteons represent its fibres and interstitial bone its matrix.

Few finite-element (FE) models have been developed to investigate the effect of micro-structural constituents on the deformation and fracture behaviour of a cortical bone tissue. Prendergast and Huiskes [16] modelled numerically an osteon to investigate the relationship between damage formation and local strain to ascertain that microdamage changes the local strain fields in the bone microstructure. Dong et al. [17] used a generalized self-consistent method to estimate the effective elastic moduli of a fibre-reinforced composite, and the model was considered useful to examine the dependence of the elastic properties of cortical bone on its porosity. In another study, Budyn and Hoc [18] introduced a multi-scale method for modelling multiple crack growth in a cortical bone tissue under tension using X-FEM. In another attempt, a micro-finite-element model of the osteonal cortical bone tissue was developed by Raeisi Najafi et al. [19] to evaluate the interaction between osteons and microcracks. The effect of cement lines on microcrack propagation paths and on the macro-scale behaviour as well as relating it to that of a homogenised material and a composite model of osteonal cortical bone tissue without cement lines can promote our understanding of their role in inhibiting bone fracture. To achieve this, a 2D micro-structural finite-element model is suggested to investigate the effect of micro-structural constituents, particularly cement lines, on fracture scenarios and the global macroscopic mechanical behaviour. This study focuses on the failure process of a micro-structural osteonal cell of cortical bone tissue using X-FEM implemented into the finite-element code Abaqus 6.10.

2. Materials and methods

2.1. Model geometry

A micro-structural cell of secondary osteonal cortical bone is simulated using three models: homogeneous, three-phase composite and four-phase composite. At micro-structural scale four different constituents are considered: osteons, interstitial bone, cement lines and Haversian canals. Osteons are considered as fibres since they are approximately circular; interstitial bone is considered a matrix as it fills the gaps between the osteons. Each osteon is surrounded by a thin layer – cement lines – and contains a canal, see Fig. 1c. The four-phase model accounts all the micro-structural types, while the three-phase composite model neglects the effect of cement lines. In this model, a constitutive behaviour of interstitial bone was assigned also to the cement-line regions. Several light-microscopy images for a radial-transverse section of the bovine cortical bone were captured from its medial position; a sample picture is shown in Fig. 1a. Those images were used to quantify geometrical parameters of the Haversian system: diameters of osteons and Haversian canals and cement lines thicknesses. All the images have identical dimensions of 0.7 mm × 0.525 mm (width × height). The statistical analysis for those images produced an osteons volumetric fraction of approx. 60% and a porosity ratio between 1.6% and 5.3%. The average width of the cement lines was between 1 and 5 μm. In the developed model, the area, directly reflecting micro-scale information, was embedded into the region with homogenised properties of the cortical bone making the dimensions of the entire model 0.9 mm × 0.725 mm × 0.3 mm (width × height × thickness). This homogenised area enabled the application of uniform external deformation and reaction forces at both cell sides. All the parameters were measured from those images using the digital image analysis software, Image-Pro Express [20]. The data obtained from that analysis were statistically analysed to be fitted to one of the well-known distributions describing the random phenomena. It was found that the random distribution of the osteons diameters can be fitted with the hypersecant distribution curve described by the values of continuous scale μ and location parameter σ –35.3 and 99.9, respectively. On the other hand, the Dagum (4P) curve revealed a good fit for the Haversian canal diameters and can be defined by $k = 1.52$, $\alpha = 2.7$, $\beta = 12.9$, and $\gamma = 3.3$.

The probability density function of the hypersecant distribution is as follows:

$$f_{hs}(x) = \frac{sech\left(\frac{\pi(x-\mu)}{2\sigma}\right)}{2\sigma} \quad (1)$$

where μ and σ are the continuous location and scale parameter, respectively.

The probability density function of Dagum (4P) distribution is as follows:

$$f_D(x) = \frac{\alpha k\left(\frac{x-\gamma}{\beta}\right)^{\alpha k-1}}{\beta\left(1+\left(\frac{x-\alpha}{\beta}\right)^{\alpha}\right)^{k+1}} \quad (2)$$

where k and α are continuous shape parameters, and β and γ are continuous scale and locations parameters, respectively.

The average diameters of osteon fibres and Haversian canals were 99.89 μm and 23.1 μm, respectively. The random microstructure of the model, Fig. 1c, was established using Matlab [21]. Using a developed script, the positions and diameters of osteons were chosen randomly based on the hypersecant distribution curve until they filled 60% of an area with the same dimensions as micrographs. Then, the Dagum (4P) distribution curve was used to choose randomly the Haversian canal diameters until their total area was within the range 1.6–5.3%. Random positions, osteons and Haversian canal diameters were then used as an input to Abaqus 6.10 [22].

2.2. Mechanical properties

In this study, the material properties of micro-structural constituents and homogenised properties of osteonal cortical bone were obtained experimentally. All the data were measured for fresh bovine diaphysis femora. Regarding the homogenised material properties, the data was based on our experimental measurements [23]. Also, the elastic data of osteons and interstitial bone were obtained using the nanoindentation technique [24]. As shown by Lakes and Saha [25], cement lines have isotropic viscoelastic behaviour due to their specific chemical composition. Therefore, its elastic properties differ from those of the osteons that they encircle. In this study, the elastic properties of cement lines were taken 25% lower than those for osteons following Budyn and Hoc [18]. Osteons, interstitial bone and cement lines were cho-